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A RE-EXAMINATION OF THE THEORY OF THE THERMAL ACCOMMODATION COEFFICIENT

by

D. M. Gilbey

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R O Y A L   A I R C R A F T   E S T A B L I S H M E N T

(FARNBOROUGH)

A RE-EXAMINATION OF THE THEORY OF THE THERMAL
ACCOMMODATION COEFFICIENT

by

D. M. Gilbey

SUMMARY

Existing theories of the accommodation coefficient for the transfer of
energy between a monatomic gas and a solid are re-examined and reconciled
with each other. Particular attention is given to the regime of high
temperatures and energies, which is of present interest in the study of high
speed flight through rarefied gases. A study is also made of other simplfied
models, showing that although the older theories can now be reconciled and
understood in simple qualitative physical terms, these theories share a number
of defects, and there is work yet to be done.

LIST OF CONTENTS

This paper comprises an examination of existing theories of the accommodation coefficient for the transfer of energy between a monatomic gas and a solid. In particular the physical bases and implications of the theory of Devonshire[1] are examined and its limitations discussed. The need for extension of the theory is established, and successive papers of this series will make some of the necessary improvements.

1   INTRODUCTION

A solid surface may have a temperature T_s differing from that (T_g) of a gas in contact with it. The gas molecules then strike the solid at a temperature T_g and leave again with some intermediate temperature T'_g, if a temperature can be assigned to the resulting energy-distribution. The thermal accommodation coefficient (α) may then be defined:

$$\alpha(T_s) = \lim_{T_g \to T_s} \frac{T'_g - T_g}{T_s - T_g} .$$ (1)

In free-molecule and slip-flow conditions, the accommodation coefficient plays a large part in determining the rate of heat transfer from a gas to a solid. We shall be concerned here with monatomic gases only, so that internal degrees of freedom will not be considered. Also, to avoid the attribution of temperature to non-equilibrium energy distributions, α will be taken to mean the coefficient for the accommodation of average kinetic energy.

2   SHORT REVIEW OF EXISTING THEORIES

The theoretical problem involves the equation of motion for a gas atom approaching and then departing from a crystal lattice. The three major areas in which simplifying assumptions are made in order to obtain a viable theory are thus

(i)   The motion of the gas atom.

(ii)   The geometrical arrangements of lattice and gas atom and the interaction forces.

(iii)   The motion of the solid lattice.

The earliest theory of the accommodation coefficient is that of Baulé[2], who assumed a hard-elastic-sphere or 'billiard ball' interaction between the gas atom and any lattice atom which it strikes. The lattice atoms were taken to vibrate about their equilibrium positions as in the Einstein specific heat model. Any gas atom which after its first encounter is still moving toward the lattice is assumed to be accommodated completely. This crude classical (as distinct from quantum) theory mainly serves to show the importance of the ratio of the mass m of the impinging gas atom to the mass M of the lattice atoms. The relevant energy-transfer factor is the familiar $4 mM/(m + M)^2$, and the resulting accommodation coefficient is independent of temperature. A merit of Baulé's theory is that he was able to consider the different possible geometrical arrangements between the gas and lattice atoms at the moment of impact: This has proved quite impracticable in the later theories, and when a lattice is considered at all, the gas atom is assumed always to approach a 'target' atom in the surface along a perpendicular to the surface passing through the target atom centre and to recede along the same line.

A more refined classical theory due to Landau[3] appeared in 1935. The lattice was replaced by a continuum, the gas atom was assumed to move in a potential $V = e^{-x/a}$ where x is the distance from the equilibrium position of the free surface, the motion of the gas atom was assumed to be unaffected to

a first order by the motion of the free surface so that for a given speed of approach the force exerted by the atom on the surface was known as a function of time, and the energy exchanged with each normal mode (plane stress wave) of motion of the continuum could be calculated by considering the amplitude and frequency with which that normal mode moved the free surface. He obtained

$$\alpha = \frac{A}{M\sqrt{m}} \left(\frac{8\pi\hbar^2 \kappa^2 T}{k\theta^2} \right)^{3/2} \tag{2}$$

where $\hbar = h/2\pi$, h is Planck's constant, T the temperature, k is Boltzmann's constant and θ is the Debye temperature. The constant A was given by Landau as $\frac{1}{4}$, but on the basis of treating the continuum in one place as a solid and otherwise as a liquid. Devonshire[1] amended A to $\frac{3}{4}$ to correct this inconsistency. The result is only valid for small α because of the perturbation method used. Also there exists no possibility of adsorption on this model because the assumed gas/solid interaction is repulsive at all distances. The range of validity of the formula is restricted because at high temperatures α becomes too large while at low temperatures the quantisation of the normal modes is important.

Devonshire in 1937 produced a quantum theory[1] of the accommodation coefficient, which corrected, superseded or included as special cases, all the previous theories. The gas atom, incident upon a target atom in the lattice was assumed to move in a Morse potential

$$V = D(e^{-2\kappa x} - 2e^{-\kappa x}) \tag{3}$$

where x is the separation between the gas atom and the target atom (minus the equilibrium separation), and D is the "well-depth" or depth of the minimum of the V(x) curve below V(∞). It is, apart from the zero-point energy, the adsorption energy. The possibility of the gas atom becoming trapped in the energy well was treated as a separate issue, and Devonshire's formula for accommodation coefficient refers to the energy exchanged by those gas atoms only which immediately bounce off the solid surface. First-order perturbation theory was used to calculate the probability of energy transfer to any one normal mode of the lattice, and summation over a Debye distribution of normal modes gave

$$\alpha = \frac{3}{\nu_m^3} \int_0^{\nu_m} \frac{\left(\frac{h\nu}{kT}\right)^3 \nu^2 \, d\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1} \int_0^{\infty} \frac{8\pi^4 m}{\kappa^2 h^2} \frac{m}{M} \frac{\sinh 2\pi\mu \, \sinh 2\pi\mu'}{(\cosh 2\pi\mu' - \cosh 2\pi\mu)^2} \frac{(A_\mu + A_\mu')^2}{A_\mu A_\mu'} e^{-\frac{E}{kT}} dE$$

$$\dots \tag{4}$$

with

$$\mu \equiv \frac{\sqrt{2mE}}{\kappa\hbar} \; ; \quad \mu' \equiv \frac{\sqrt{2m(E+h\nu)}}{\kappa\hbar} \; ; \quad d \equiv \frac{\sqrt{2mD}}{\kappa\hbar}$$

and

$$A_\mu \equiv \left| \Gamma(-d + \tfrac{1}{2} + i\mu) \right|^2 \quad (i \equiv \sqrt{-1}) \quad .$$

$$\tag{5}$$

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Here the symbols have their previous significance, ν is a normal-mode frequency, ν_m is the Debye maximum frequency and E is the initial kinetic energy of a gas molecule. A misprint of ν_m^2 in place of ν_m^3 occurs twice in the original paper. The effects of a simple exponential repulsive interaction may be obtained as the limit of equation (4) as $D \to 0$ i.e. $d \to 0$ and the corresponding accommodation coefficient is

$$\alpha \;=\; \frac{3}{\nu_m^3} \int_{0}^{\nu_m} \frac{\left(\frac{h\nu}{kT}\right)^3 \nu^2 \, d\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1} \int_{0}^{\infty} \frac{8\pi^4_m}{\kappa^2 h^2} \; \frac{m}{M} \; \frac{\sinh \pi\mu \, \sinh \pi\mu'}{(\cosh \pi\mu' - \cosh \pi\mu)^2} \; e^{-\frac{E}{kT}} \, dE \; .$$

$$\ldots (6)$$

Devonshire points out that with the approximations $\mu\pi \gg 1$, $E \gg h\nu$, and $kT \gg h\nu$, formula 6 can be reduced to Landau's expression 2, but only if the integrand of 6 is small for $\nu > \nu_m$ and then A is found to be $\frac{3}{8}$, not $\frac{3}{4}$.

The above approximations are valid at high temperatures except that unfortunately, the condition on the integrand is only valid at low temperatures, when it becomes so because of quantisation of the lattice vibrations and because the "duration of collision" between gas atom and lattice becomes large.

In the course of obtaining equation (4), Devonshire assumes that κ times the amplitude of thermal motion of the target atom is small, and that the interaction energy between the gas atom and the lattice is a function only of the separation between target and gas atoms. The interaction potential V is then represented, if z and u are the coordinates of target and gas atom respectively, by

$$V(u,z) \;\simeq\; V(u,0) - z \frac{\partial V(u,0)}{\partial u} \qquad (7)$$

$$V(u,0) \;=\; D\left[e^{-2\kappa u} - 2e^{-\kappa u} \right] \; . \qquad (8)$$

Because the approximation 7 is linear in z, and because z is linear in the normal coordinates for the crystal vibrations, it follows[4] that in the first-order perturbation scheme, only one normal mode can change its quantum number, and that by only ± 1. The integration over all normal modes in 4 is therefore only justified if the sum of the one-quantum transition probabilities is much less than one, because the integration assumes complete independence of the probabilities for each normal mode, whereas in the first-order theory used, if one normal mode exchanges a phonon, this prevents any other mode from doing so. The sum of transition probabilities is the same integral as 4, but with the integrand first divided by $(h\nu/kT)$. It follows that at high temperatures, or when α becomes large, formula 4 may give an over-estimate of the accommodation coefficient which should result from first order theory.

This becomes obvious when calculations according to 4 are made; values of α can be obtained which necessarily imply the exchange of many phonons.

Landau[3] pointed out that for higher temperatures and heavier gas atoms, classical mechanics must give a good approximation to the truth. That his theory is invalid for high temperatures is mainly because he incorrectly

assumed that his finite integral over normal modes could be approximated by an infinite one. Recently, Zwanzig[5] has also suggested that a classical approach must be used to handle the large energy-transfers which must be expected at high temperature. He made a study of a one-dimensional model for the solid, consisting of discrete masses connected by springs, with the gas "atom" incident upon the end of the chain and interacting with the last "solid atom" according to various potentials. Large accommodation coefficients were derived. Bonch-Bruevich[6] has complained that the complexity of the mathematical formulation of the results obtained in the series of papers by Lennard-Jones, Devonshire, and Strachan completely obscures any physical insight and makes the theory too difficult to apply. There may be some justification for this, since writers on problems concerning high speed aviation use[7] Baulé's theory in any consideration of accommodation coefficient, despite its obvious naivety. Later in this paper the qualitative physical features and consequences of the Devonshire theory will be exhibited clearly.

3   RECONCILIATION OF THE THEORIES

In this section a high-temperature approximation to the theories of Landau and of Devonshire will be derived and related to the simple Baulé concept of classical collisions between hard spheres. The factor of two between Landau and Devonshire persists in this regime and an examination of simple one-dimensional models reveals that this factor is a measure of the inadequacy of a continuum model for the representation of the higher-frequency motions of a lattice. It is also shown that the Devonshire theory, although correct in the high temperature limit, does not lead in general to a correct distribution of the exchanged energy among the normal modes of the crystal.

If in formula 6 the approximations $\mu\pi \gg 1$, $E \gg h\nu$, $kT \gg h\nu$ are made, which are appropriate to high temperatures or high energies in the oncoming gas atoms, but no assumption is made as to the magnitude of the integrand for $\nu > \nu_m$, then (9) is obtained:

$$\alpha = \frac{3}{\nu_m^3}\ \frac{m}{M}\ \frac{8\pi^4 m}{\kappa^2}\ \frac{1}{(kT)^2} \int_0^{\nu_m} \nu^4\,d\nu \int_0^\infty \frac{e^{-E/kT}\,dE}{4\sinh^2(\pi^2 m^{\frac{1}{2}}\nu/\kappa E^{\frac{1}{2}} 2^{\frac{1}{2}})} \,. \qquad \ldots\ (9)$$

Devonshire's repulsive potential is $e^{-2\kappa x}$ (see equation (8)), whereas Landau uses $e^{-x/a}$, so we may put $\kappa = 1/2a$. Also if V_z is the speed of approach of the gas atom toward the solid, then $\frac{1}{2}mV_z^2 = E$. The formula (9) is of the form

$$\alpha = \int_0^{\omega_m} n(\omega) \int_0^\infty \frac{e^{-E/kT}\,dE}{(kT)^2} G(E,\omega) \qquad (10)$$

where $G(E,\omega)$ is the average energy given by the gas atom to each of the normal modes whose periodicity is $\omega = 2\pi\nu$, the integral over E is to average over the various energies which the gas atom can have and $n(\omega) = 9\,N\omega^2\,d\omega/\omega_m^3$ defines the distribution of frequencies among the normal modes. N is the number of atoms in the crystal and

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$$G(E,\omega) \quad = \quad \frac{2\ m^2 \pi^2 \omega^2 a^2}{3\ NM\ \sinh^2(\pi \omega a/v_z)} \tag{11}$$

which is once again just one-half of the value obtained by Landau.

At this stage we may note in passing that if $\pi \omega_m a \gg \sqrt{(2kT/m)}$, then G and the integrand of 10 are very small for $\omega > \omega_m$, and we may extend the integral over ω to infinity, as Landau did, without error. Physically, this means that energy is transferred only to low-frequency modes because only low frequencies appear significantly in the harmonic analysis of the force exerted by the gas atom on the lattice when the gas atom has a small kinetic energy. This holds approximately for low temperatures. If the temperature is too low however, the approximation $\mu\pi \gg 1$ breaks down, which means that even the motion of the gas atom is significantly quantised. In all of this the attractive force between lattice and gas atoms has been omitted.

A more interesting regime for our present purpose is that of high temperature, when the approximation $\pi \omega_m a \ll \sqrt{(2kT/m)}$ is appropriate. It is then easily shown that the integrand in 10 is only significant when $\pi \omega a/v_z$ is small, so that the sinh function may be replaced by its argument. The result, from (11), is

$$G \quad = \quad \frac{2\ m^2 v_z^2}{3NM}\ ; \quad \alpha \quad = \quad \frac{4m}{M} \tag{12}$$

showing that in this limit every mode receives an equal share of energy (after the implied averaging over the angles θ between the direction of motion of the gas atom and the direction of motion of the lattice atom engendered by the various normal modes of approximately the same frequency). This is because the force exerted by the gas atom on the lattice is now essentially impulsive, contributing equal amplitudes for its harmonic components at all frequencies, and the "effective mass" for each normal mode oscillator is 3 NM. The factor 3 arises because the average of $\cos^2\theta$ for the three normal modes (2 transverse and 1 longitudinal) associated with each possible wave-number vector is $1/3$. The total number of vibrational modes is nearly 3N and NM is the total mass of the crystal. Since the gas/solid interaction becomes impulsive at high gas atom energies, only the target lattice atom plays any role in the energy transfer, provided m < M so that only one collision occurs. Thus classically one would expect in this limit $\alpha = 4\ mM/(m + M)^2$. The result (12) is the approximation to this for m $\ll$ M, which is to be expected since α was assumed small in both the Landau and the Devonshire theories.

It is nevertheless surprising at first sight that the first-order wave-mechanical perturbation theory should give essentially the correct answer for this 'classical' limit of high energies. At the same time the classical theory of Landau gives $\alpha = 8\ m/M$, which is obviously wrong. It should be noted also that while (12) is only correct if α is small, nevertheless at high temperatures the exchange of many phonons is predicted, which contradicts the argument forcibly made by Zener[4], and apparently accepted by Devonshire[1] and Strachan[8], that only one normal mode can change its quantum number and that by only ±1 because of the harmonic oscillator selection rules. It can be shown, with the expense of considerable manipulation, that the limiting form (12) for the Devonshire theory remains true

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in principle even when the attractive potential in (8) is retained. This is to be expected physically since at sufficiently great thermal energies (kT), the well-depth D will become negligible in comparison. For a well-depth of several kilocals/mole or more, the high-temperature limit is experimentally unattainable as the solid will melt or vapourise. It is of interest, though, for the consideration of the impact of fast molecules upon cold surfaces, such as happens when an artificial earth satellite collides with molecules of the upper atmosphere. Numerical calculations of α from equation (4) are presented in Fig.1.

It will now be shown that Devonshire's integration over modes is correct, not an approximation, at high temperatures, and that given the integration, the first-order perturbation theory should give the correct classical result in this regime, as it in fact does. The following argument is limited to high temperatures by the proviso that the gas atom may be replaced by a time-dependent force on the target lattice atom and that the force should be unrelated in phase to any particular lattice vibrations and independent of any transitions caused in the lattice. This implies that α is small and that $kT \gg \hbar\omega_{max}$.

Consider a crystal comprising N point-mass atoms interlinked by perfect Hooke's-law springs. For convenience let the crystal be attached by other springs to a rigid support in such a way that it cannot rotate or translate indefinitely. All the 3N normal modes of the system will then be vibrations at non-zero periodicities ω_r where $1 \leqslant r \leqslant 3N$. We may define a symmetrical mass-matrix, which in our case will be M times the unit matrix of order 3N and will be denoted by M. Whether M denotes the scalar or the matrix can be judged from the context in what follows. A symmetrical stiffness matrix S may also be formed and if X is the vector of the 3N displacements of the N atoms from their equilibrium positions, the equations of motion of the crystal under no external forces may be written

$$M\ddot{X} + SX = 0 . \qquad (13)$$

Consideration of this shows that the eigenvalues of $M^{-1}S$ are ω_r^2, which may be formed into a diagonal matrix W. The corresponding eigenvectors may be considered the columns (known as modal columns) T_r of a matrix T. The linear transformation $X = TQ$ introduces the vector Q of normal coordinates, $M^* \equiv T'MT$ is the diagonal matrix of normal mode effective masses (chosen so that the kinetic energy $\frac{1}{2}\dot{X}'M\dot{X}$ becomes $\frac{1}{2}\dot{Q}'M^*\dot{Q}$ in the new coordinates), and the equations of motion become

$$M^*\ddot{Q} + M^*WQ = 0 . \qquad (14)$$

The columns T_r of T are so far arbitrary to the extent of a multiplicative constant. These constants may be chosen so as to make M^* the unit matrix if desired.

The introduction of a vector F(t) of time-dependent forces, which must be independent of the positions of the atoms, on the right-hand side of equation (13) gives:

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$$M\ddot{X} + SX = F(t) \tag{15}$$

$$M^*\ddot{Q} + M^*WQ = T'F(t) \ . \tag{16}$$

A point to be made immediately is that the last equation comprises 3N completely independent equations, one for each of the components q_r of Q, since the matrices M^* and W are diagonal; each is an equation for the motion of single oscillator with an external force applied. This statement applies equally to the quantum mechanical formulation and, provided the initial phases of the various normal mode oscillators bear no particular relation to each other or to the timing of the applied force, it follows that the normal modes absorb energy from the applied force independently. In other words, the probability that one of the normal modes changes its quantum number from n_r to n_r' is independent of any transition that any other normal mode may make. This directly contradicts the statements by Zener and others, arising from the use of first-order perturbation methods, that a quantum-mechanical selection rule operates so that only one normal mode may change its quantum number, and that by ± 1.

It is also interesting to note[9] that the average energy uptake by a quantum oscillator of random initial phase (i.e. definite energy) is the same as for a classical oscillator, and is independent of the initial energy. Thus in the regime considered, i.e. when the gas atom may be replaced by a force varying in time but independent of the position of the target lattice atom, α must be the same whether calculated classically or by quantum mechanics. This is true both for multiphonon energy transfer and for conditions when first order perturbation theory is valid. Obviously however, $h\nu$ must be considerably less than kT for the interaction force to be a given function of time, i.e. independent of whether or not a transition occurs. Similarly, α must be small, but this is a limitation of both types of theory, and does not imply that multiphonon transfers do not occur.

So far in this section arguments have been given to show that, at least for high temperatures, the integration over normal modes in Devonshire's theory is the correct procedure and not an approximation as previously assumed. As Strachan has pointed out in some detail, the probability of a single mode exchanging more than one phonon is very small because the exchanged phonons are shared among 3N modes, where N is a large number. It follows that first order perturbation theory should give correct answers even at high temperatures for the individual transition probabilities. This regime of high temperature, low α, will now be considered in more detail.

Equation (16) may be written as a set of equations:

$$M_r^* \ddot{q}_r + M_r^* \omega_r^2 q_r = f_r(t) \tag{17}$$

where $f_r(t)$ is the r'th component of $T'F(t)$. Let n_r be the initial quantum number (at $t = -\infty$) of the r'th mode and n_r' the final quantum number (at $t = \infty$). Goldman[9] et al have given formulae for the transition probabilities $P(n_r, n_r')$ of a system described by equation (17), and it may easily be shown from their work that

$$P(n_r, \, n'_r) \;=\; \left| \left[\exp(ik_r \, q_r) \right]_{n_r \, n'_r} \right|^2$$

where

$$k_r^2 \;=\; \omega_r \left| \int_{-\infty}^{\infty} f_r(t) \, \exp(i\omega_r t) \, dt \right|^2 \Big/ \hbar \;\equiv\; \omega_r \left| F_r(\omega_r) \right|^2 \Big/ \hbar$$

and

$$\left[\exp(ik_r \, q_r) \right]_{n_r n'_r} \;\equiv\; \int_{-\infty}^{\infty} \psi_{n'_r}^*(q_r) \, \exp(ik_r \, q_r) \, \psi_{n_r}(q_r) \, dq_r \; .$$

... (18)

Here ψ_{n_r} is the n'_rth normalised harmonic oscillator eigenfunction.
Returning to the complete system, we may denote by $P(n,n')$ the probability
that the vector n of the n_r will change to a vector n', and since the
individual probabilities are independent,

$$P(n,n') \;=\; \prod_r P(n_r, \, n'_r) \;=\; \left| \left[\exp\!\left(\sum_r ik_r \, q_r \right) \right]_{nn'} \right|^2$$

$$\left[\exp\!\left(\sum_r ik_r \, q_r \right) \right]_{nn'} \;\equiv\; \int_{-\infty}^{\infty} \psi_{n'}^* \, \exp\!\left(\sum_r ik_r \, q_r \right) \psi_n \, dq$$

$$\psi_n \;\equiv\; \prod_r \psi_{n_r}(q_r) \; ; \qquad dq \;=\; \prod_r dq_r \; ; \; r = 1(1)3N \; .$$

... (19)

As mentioned above, owing to the great number of modes, the
individual transition probabilities are all very small (for non-zero
energy exchange) though their total may be large. In other words $k_r \, q_r$

is small but $\sum_r k_r \, q_r$ may be large. $f_r(t)$ in equation (17) is small

because it is a component of $T'F(t)$ and in our problem, only one component
of $F(t)$ is non-zero; we are trying to excite a vibration involving all the
atoms of the crystal by pushing on only one of them. The first order
perturbation expression for $P(n_r, \, n'_r)$ may be obtained by expanding the
exponential in equation (18),

$$P(n_r, n_r') \simeq \left| \left[1 + ik_r \ q_r \right]_{n_r, n_r'} \right|^2$$

$$= \delta_{n_r, n_r'} + \frac{|F_r(\omega_r)|^2}{2M_r^* \ \hbar \omega_r} \left[n_r \ \delta_{n_r, n_r'+1} + (n_r + 1) \ \delta_{n_r, n_r'-1} \right] , \qquad (20)$$

which exhibits the well known selection rule for first-order perturbations in that n_r can change at most by ± 1. It may also be noted that the average energy absorbed by the r'th oscillator is just $|F_r(\omega_r)|^2/2M_r^*$, the classical value. This has been noted[10,11] in other contexts. The interesting fact is that the first order result for energy transfer is valid to all orders as it coincides with the classical result and therefore with the result of the exact quantum theory. For large energy transfers, the exact theory would give a widespread spectrum of final states whereas the first-order theory would give a large (greater than unity!) probability of exciting the two states adjacent to the initial state; the energy transfer would nevertheless be the same. Thus for the system under discussion, first order perturbation calculations of energy transfer are correct even when multiphonon transitions of a single oscillator occur. We do not need this result, but we are concerned about the probability of several oscillators each transferring a single quantum.

The average overall energy transfer ΔE is

$$\Delta E = \sum_{n'} P(n,n') \sum_r (n_r' - n_r) \hbar \omega_r \equiv \sum_{n'} P(n,n') \sum_r E_r(n_r, n_r') .$$

$$\dots (21)$$

With the use of (19) this can be rewritten

$$\Delta E = \sum_{n'} \left[\prod_r P(n_r, n_r') \right] \left[\sum_r E_r(n_r, n_r') \right] .$$

Remembering that $\sum_{n_r'} P(n_r, n_r') = 1$ and that $P(n_r, n_r')$ and $E_r(n_r, n_r')$ are independent of all components of n' save n_r', this can be reduced to

$$\Delta E = \sum_r \sum_{n_r'} P(n_r, n_r') \ E_r(n_r, n_r') , \qquad (22)$$

which is equivalent to Devonshire's integration over modes and shows (if it needed demonstration) that energy transfer to one mode is independent of transfer to other modes. It remains to see how first order perturbation

theory can lead to Zener's conclusion that the modes are not independent:
First order perturbation theory is equivalent to retaining only the terms

linear in k_r in the expansion of $\exp\left(\sum_r ik_r q_r\right)$, and far more disastrously,

neglecting all products such as $k_r k_s$. One then obtains from (21) and (19):

$$\Delta E = \sum_{n'} \left| \left[1 + \sum_r ik_r q_r\right]_{nn'} \right|^2 \sum_r E_r(n_r, n'_r)$$

$$= \sum_{n'} \sum_r k_r^2 [q_r]_{nn'}^2 E_r(n, n')$$

which involves the sum of terms such as occur in equation (20), but each
multiplied by $\pm\hbar\omega_r$ or zero. From this formulation, Zener's conclusions
follow, but the 'selection rules' are now seen to be a defect of the
first-order approximation and not a reality.

In view of the foregoing we may deduce that on the questions so far
covered the Devonshire formula should give correct accommodation coef-
ficients α for both large and small energy transfers, provided α is itself
small; within this restriction it agrees with classical theory for high
temperatures. The problem remains of the incorrect factor of 2 in Landau's
working. To show the reason for this it is necessary to consider the
normal modes of the solid in more detail. For this particular purpose,
classical one-dimensional models suffice. The model of a linear chain
of similar atoms with nearest-neighbour Hooke's law interaction is con-
sidered in Appendix 1, also the model of a linear continuum (rod) with a
'Debye' cutoff of normal mode frequencies. In the second model the end
of the rod always vibrates at maximum amplitude no matter which normal
mode is excited, and the equivalent mass of the normal mode, determined
from the energy of the whole rod for unit amplitude displacement of the
end, is always just one half of the total mass of the rod. In the model
with discrete masses the amplitude of the end atom for a given energy in
the chain decreases with increasing frequency of the normal mode and the
equivalent mass of the n'th mode oscillator is $NM/2 \cos^2(n\pi/2N)$, where NM
is the total mass and N the total number of atoms in the chain. Since the
energy transferred to a mode is inversely proportional to the effective
mass it is obvious that excitation of the higher frequency modes is not so
easy for the chain of discrete masses as for the continuum. When an
impulse is delivered to the end atom all modes receive an equal impulse
and the average value of $\cos^2(n\pi/2N)$ for $n = O(1)N-1$ is $1/2$, so that the
chain absorbs only half the energy taken up by the continuum. This is the
source of Landau's mistake. Devonshire actually treats the surface atom
as though it were in the middle of an infinite lattice and takes in effect
NM as the mass of every mode. This gives the right answer for the impul-
sive force, but for forces distributed over a time interval it will not
give the true preference for excitation of lower frequency modes. It will
be shown later that one-dimensional models give erroneous results for
accommodation coefficients, but they do serve to illustrate the above
difference between lattices and continua.

4   SIMPLE CONTINUUM MODELS

A one-dimensional (1D) continuum rod has been considered in Appendix 1 from the point of view of its normal modes. It is easy to show that in a perfectly elastic 1D continuum with no dispersion or "Debye cuttoff", any energy supplied at one end is radiated as an unchanging stress wave down the rod; any work done by a force on the end of the rod is lost forever to the agency responsible for the force if the rod is infinitely long. Introduction of the dispersion proper to a lattice of like atoms connected with Hooke's law springs to nearest neighbours only does not greatly alter the situation. The 1D infinite chain has been considered in some detail by Zwanzig, and is found to give large accommodation coefficients, as expected, unless the impinging atom is much lighter than the lattice atom. In the latter event only the 'target' atom in the chain plays any significant role and Baulé's factor applies since the collision is over before the target atom has moved sufficiently to affect the rest of the lattice.

In this section a very naive 3D continuum model will be used to highlight the inadequacy of 1D models, and a more sophisticated 3D model, available from the work of Miller and Pursey[12],[13] on waves in the earth's crust, will show the importance of surface waves.

Firstly let us consider a (non-physical) 3D continuum in which the free surface is the plane $\theta = \pi/2$ in spherical polars and the medium is in the region $0 \leqslant \theta \leqslant \pi/2$. Suppose that the displacement s of the medium parallel to $\theta = 0$ can be completely decoupled from any displacement in any other direction and that it obeys the wave equation

$$\lambda \nabla^2_s = \rho \ddot{s} \tag{23}$$

where λ is an elastic modulus and ρ the density. If we do not concern ourselves with the boundary conditions at $\theta = \pi/2$, hemispherical scalar waves are possible with no dispersion so that

$$S(r,t) = \frac{r_o}{r} S\left(r_o, \ t - \frac{r - r_o}{c}\right), \quad c^2 = \lambda/\rho . \tag{24}$$

Also in this model the stress transmitted across unit area of the hemisphere $r = r_1$ is $\lambda \frac{\partial s}{\partial r}$, giving a total force F between the regions on either side of the hemisphere, and

$$F = 2\pi r^2 (\partial s/\partial r)_t \cdot \lambda . \tag{25}$$

We now consider that the force between an oncoming body of mass m and the continuum is applied to the continuum over the hemisphere $r = r_o$. Making use of (24) and (25) we have

$$m\ddot{s}(r_o) = F(r_o) = -2\pi\lambda\left[r_o^2 \dot{S}(r_o)/c + r_o S(r_o)\right] . \tag{26}$$

In the square brackets on the right hand side of (26), the first term is a damping term arising because any disturbance of the medium at $r = r_o$ causes a wave to be radiated. This first term appears in the equations for the 1D model, but in the latter there is no counterpart to the second term. The second term represents a conservative restoring force connected with the steady-state solution $S(r) = (r_o/r) S(r_o)$ of (24). The 1D continuum has no steady-state solution. Thus the 3D continuum behaves mechanically, for a force applied at $r = r_o$, like a spring of force constant $2\pi \lambda/r_o$ (conservative part) in parallel with a dashpot (wave-making resistance). The differential equation (26) for $s(r_o)$ is the well-known equation for damped oscillations, and may be solved with initial conditions $\dot{s} = v_o$, $s = 0$, to find v_1, the final velocity of the oncoming mass at the time when $\ddot{S}(r_o)$ returns to zero. Putting $\alpha = 1 - v_1^2/v_o^2$ then gives for this model

$$\alpha = 1 - \exp(-4\theta \cot \theta) \qquad (27)$$

where $\tan \theta = -\sqrt{\left[\left(2m/\pi \rho r_o^3\right) - 1\right]}$. We may roughly identify ρr_o^3 with the mass M of the lattice atom, and it is then clear that this model suggests the possibility of very poor accommodation when m/M is large. The physical reason for this is that a heavy oncoming atom distorts the solid relatively slowly, losing very little energy to lattice waves, being finally brought to rest and then catapulted from the solid by the conservative or "steady state" forces set up by the distortion. This possibility does not exist in 1D because there is no "steady state" force. Also it is not comprehended in the perturbation theories of Devonshire and of Landau, which predict for $m \gg M$ that $\alpha > 1$ because the perturbation method is not valid in this regime. Zwanzig, in his consideration of a 1D chain also suggests that $\alpha = 1$ for $m > M$ because then the oncoming atom is still moving into the chain after its first collision and will therefore suffer multiple collisions with the target atom in the chain. There is a general consensus that multiple collisions lead to perfect accommodation. This is true of Zwanzig's model, but the simple 3D model outlined above suggests that it is not true for a 3D lattice. This expectation has been justified in the work[14] of F.O. Goodman on classical lattice dynamics.

The above discussion shows the inadequacy of 1D models. We now turn to the shortcomings of existing 3D models for accommodation coefficient theories. Miller and Pursey[12] have considered an isotropic elastic continuum bounded by a flat stress-free surface except that over a disc of radius a in this surface a uniform pressure is applied with sinusoidal time-dependence. They have solved the problem using integral transforms for a general value of Poisson's ratio and for the mean displacement over the disc in the direction normal to the surface, $\bar{U}_z$, they obtain

$$\bar{u}_z = \frac{2 \mu^2 p}{k_1 C_{44}} \int_0^\infty \frac{\sqrt{(\xi^2 - 1)} \, J_1^2(\xi a k_1) \, d\xi}{\xi F_o(\xi)} \qquad (28)$$

where k_1 is the wave number for the longitudinal waves generated in the medium, μ is the ratio of wave speeds $\dfrac{\text{longitudinal}}{\text{transverse}}$, p is the pressure applied, C_{44} is the shear modulus and F_o is a function of μ and ξ:

- 14 -

$$F_o(\xi) \;=\; (2\,\xi^2 - \mu^2) \;-\; 4\,\xi^2\,\sqrt{(\xi^2-1)(\xi^2-\mu^2)}\;. \tag{29}$$

The path of integration is to be taken above the singularities on the real axis, and the principal values of the square roots must be used. This last condition means that F_o has only one zero which gives a pole in the integrand at $\xi = \xi_o$, where $\xi_o > \mu$ on the real axis. It is the residue at this pole which gives the effect of surface waves.

Miller and Pursey, from equation (28), have made numerical estimations of the mechanical impedance presented by the continuum at the disc source. Some of the results are reproduced in Table 1.

Putting $F = \pi r_o^2\,p$, $\dot{s} = i\omega s$, $\lambda = \rho c^2$, $r_o = ak$ and $\omega/k = C$ in equation (20), it is found that the impedance is predicted by the naive 3D model to be $2\,\rho c(1 - i/a)$. In Table 1, Z_R is the radiative impedance and V_L the velocity of longitudinal waves in Miller and Pursey's model. σ is Poisson's ratio.

TABLE 1

a	$Z_R/\rho\,V_L$	
	$\sigma = 1/4$ $\mu = \sqrt{3}$	$\sigma = 1/3$ $\mu = 2$
0.05	0.66 - 10.46 i	0.64 - 8.82 i
0.10	0.66 - 5.22 i	0.64 - 4.39 i
0.20	0.66 - 2.58 i	0.64 - 2.16 i
0.30	0.67 - 1.68 i	0.65 - 1.40 i
0.40	0.67 - 1.22 i	0.65 - 1.01 i
0.50	0.68 - 0.94 i	0.66 - 0.76 i

It can be seen that for small a, i.e. when the radius of the disc is small compared to the wavelength of the elastic waves, the impedance comprises a constant resistive (wave making) part together with a reactive (capacitative) part proportional to 1/a as suggested by the naive model. The reactive part makes possible a steady state with a non-zero applied pressure. In the same limit of small a, a lattice should become comparable to the continuum.

In another paper Miller and Pursey[12] find what proportions of the energy radiated are to be found far from the source in the form of longitudinal, transverse, and surface waves. The proportions for $\sigma = 1/4$, i.e. $\mu = \sqrt{3}$, are 0.333, 1.246, and 3.257 respectively, showing that two thirds of the energy is lost in the surface wave. This suggests that existing treatments of the thermal accommodation coefficient problem may be in error by a factor of 3 or more, since energy loss to surface waves is never considered. Consideration of (29) shows that as μ tends to unity the zero of $F_o(\xi)$ tends to infinity and the pole of the integrand in (28) contributes nothing to $\bar{u}_z$;

correspondingly, as the ratio of longitudinal to transverse wave speeds tends to unity, the surface wave disappears. This limit is quite non-physical, requiring an infinite Poisson's ratio, but serves to show that surface waves cannot be expected in a model which assumes equal transverse and longitudinal wave speeds. This means that an adequate lattice model which is also amenable to mathematical treatment is difficult to find.

5 CONCLUSION

It is shown above that when the energy of the gas atoms impinging on a solid surface is sufficiently high, Devonshire's formula for accommodation coefficient reduces to $\alpha = 4\,m/M$, where m and M are the masses of gas atoms and lattice atoms respectively. This is to be regarded as an approximation to the collisional energy transfer factor $4\,mM/(m + M)^2$, valid for $m \ll M$, and shows that Devonshire's theory can successfully predict many-phonon transitions in the lattice. This unexpected success of the first order quantum mechanical perturbation theory is due firstly to the fact that the quantum mechanical oscillator behaves classically with respect to absorption of energy from a perturbing force and secondly to the integration over normal modes which assumes complete independence of the modes in the absorption of energy. While the modes are not independent in the first order perturbation theory, they would become so in a treatment valid for multiphonon transitions. Devonshire's formula is concerned with those gas atoms only which immediately leave the solid surface after impact; for correlation with experimental results, some account should be taken of those gas atoms which remain adsorbed on the solid after the impact.

In the same limit of high gas atom energies, it is shown that Landau's model gives $\alpha = 8\,m/M$ and this obviously incorrect result arises because his continuum model with a force applied at the free surface does not behave at high frequencies like a lattice. It would behave more correctly if the forces could be applied half a lattice spacing in from the continuum surface, provided the effect of the forces is calculated by Landau's perturbation method. Devonshire used a lattice model but considered the interaction of the gas atom with an atom in the bulk of the lattice instead of with an atom at a free surface. Thus although he obtains the correct result for the high energy gas atom (impulsive force) situation, at lower energies his formula will not give the correct bias towards exciting low-frequency modes.

It is also shown above that one-dimensional models are not adequate for the study of accommodation coefficients. A three dimensional solid, in contrast to a one-dimensional solid, can behave conservatively with respect to a force applied over a finite region of its free surface, provided the force changes sufficiently slowly. This leads to the suggestion that there should be poor accommodation when a very heavy gas atom impinges on a lattice of light atoms. All the existing theories, save that[14] developed by Dr. Goodman at this establishment, predict very good accommodation in this situation on the grounds that the gas atom makes more than one collision with the target atoms in the lattice, which argument ignores the "resilience" of the three dimensional lattice. Devonshire and Landau both predict high α because the energy transfer is treated as a perturbation of the situation of a gas atom impinging upon a rigidly fixed target lattice atom. It would be more realistic to start with a gas atom impinging on a perfectly restitutive lattice as a zero order solution for this particular case of large mass-ratio.

Finally, it is shown that surface waves are likely to play an important part in gas-solid energy exchange, perhaps to the extent of increasing the energy transfer by a factor of three or more.

LIST OF SYMBOLS

A	constant, equation (2)
A_s	normalising factor for s'th normal coordinate
A_μ	see equation (5)
a	scale length for exponential repulsion in Landau's theory equation (9), (10), (11). r_o/k in Table 1
a_r	coefficients, equation (13)
c	speed of elastic wave, equation (18)
C_{44}	elastic constant of solid
D	energy "well-depth", equation (3)
1-D	abbreviation for "one-dimensional"
d	see equation (5)
E	initial kinetic energy of gas molecule, equation (4)
E_s	energy in s'th mode or energy transferred to s'th mode
F	force or vector of forces applied to solid, equation (19)
$F(\omega)$	fourier component of driving force f(t), equation (16)
F_o	see equation (23)
f(t)	force applied to oscillator
G	see equation (10)
h	Planck's constant
$\hbar$	$h/2\pi$
I	Impulse
i	$\sqrt{-1}$
k	Boltzmann's constant, or $|F|/\sqrt{2m\hbar\omega}$ in equation (18) et seq., or wave-number or bond-stretching force constant in Appendix 1
k_1	wave number for longitudinal waves

LIST OF SYMBOLS (Contd)

L   length of rod (Appendix 1)

M   mass of solid atom, total mass of solid in Appendix 1

M*   effective mass of normal mode oscillator or the matrix of these

m   mass of gas atom. Mass of solid atom in Appendix 1

N   number of atoms in solid lattice

$n(\omega)$ frequency distribution of normal modes, equation (10)

P   transition probability

p   pressure

Q   vector of normal coordinates, equation (A1-3), equation (14)

r   radial coordinate in spherical polars

S   stiffness matrix

s   displacement, equation (17); normal mode number

T   temperature

T_{rs} components of matrix T in equation (A1-3) and equation (16)

t   time

u   coordinate of gas atom

$\bar{u}_z$ mean displacement, equation (22)

V   potential energy

V_L speed of longitudinal elastic waves in solid

v   gas atom velocity

X   vector of lattice atom displacements, equation (A1-3)

x   distance of gas atom from surface; displacement of target atom

Z_R radiative impedance

z   coordinate of target lattice atom

α accommodation coefficient. Equation (1)

Γ gamma function

θ Debye temperature; angle between elastic wavefront and surface;
            azimuthal coordinate in spherical polars. See also equation (21)
            and Appendix 1.

LIST OF SYMBOLS (Contd)

κ	factor determining width of potential well, equation (3)
λ	elastic modulus, equation (17)
μ	see equation (5), also ratio of elastic wave speeds in Table 1
ν	normal mode frequency
ν_m	Debye's limiting frequency
ρ	density, equation (17)
σ	Poisson's ratio (Table 1)
ψ	harmonic oscillator wave-function
ω	$2\pi\nu$

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Appendix 1
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APPENDIX 1

SIMPLE ONE-DIMENSIONAL MODELS

Consider a linear chain of N atoms each of mass m and connected to its nearest neighbours by a spring of force constant k. Let the atoms be numbered 0 to N-1, and let x_r be the displacement from its initial rest position of the r'th atom. The equation of motion of the r'th atom

$$k(x_{r+1} - 2 x_r + x_{r-1}) = m \ddot{x}_r \qquad (A1-1)$$

can be satisfied by $x_r = x_{ro} \sin \omega t \cos(r\theta + \phi)$ provided $\omega^2 = (2k/m)(1 - \cos \theta)$. The equations of motion of the atoms 0 and N-1 are also satisfied if $\phi = \theta/2$ and $\theta = s\pi/N$ where s is an integer. The displacement T_{rs} of the r'th atom when the s'th normal coordinate only is made unity is thus, with $s = 0(1)N-1$,

$$T_{rs} = A_s \cos\left(r + \frac{1}{2}\right) \frac{s\pi}{N} . \qquad (A1-2)$$

It is convenient to give A_s^2 the value 2/N for $s \neq 0$ and 1/N for $s = 0$, since then the matrix $||T_{rs}||$ is the inverse of its transpose as may readily be verified. The columns of this matrix are often referred to as 'modal columns'. If $X = \{x_r\}$ is the vector of atom displacements and Q is the vector of normal coordinates and T is written for $||T_{rs}||$, we have

$$X = TQ . \qquad (A1-3)$$

The equations of motion (A1-1) may be expressed in matrix form

$$\ddot{X} + BX = 0$$

which may be generalised, if F(t) is a vector of forces applied to the atoms, to

$$\ddot{X} + BX = \frac{1}{m} F \qquad (A1-4)$$

or

$$\ddot{Q} + TBT^{-1} Q = T^{-1}\left(\frac{1}{m} F\right) . \qquad (A1-5)$$

The matrix TBT^{-1} is diagonal with the s'th element equal to $\omega_s^2 = (2k/m)\left(1 - \cos \frac{s\pi}{N}\right)$. If in particular a force is applied to the zero'th atom only then the equations for the normal coordinates Q_s are all of the form

$$\ddot{Q}_s + \omega_s^2 Q_s = A_s \left(\cos \frac{s\pi}{2N} \right) F(t)/m \qquad (A1\text{-}6)$$

and if $F(t)$ is an impulse I applied at $t = 0$ to a chain at rest then

$$\dot{Q}_s(t = 0) = \frac{A_s I}{m} \cos \frac{s\pi}{2N} \qquad . \qquad (A1\text{-}7)$$

It can be shown from (A1-3) that the energy associated with the s'th mode is $\frac{1}{2} m \dot{Q}_s^2(t = 0)$ for $s \neq 0$ and $m \dot{Q}_o^2(t = 0)$ for $s = 0$. In any case the energy in the s'th mode after application of the impulse is

$$E_s = \frac{I^2}{mN} \cos^2 \frac{s\pi}{2N} \qquad . \qquad (A1\text{-}8)$$

The total energy in the chain is of course $I^2/2m$, the energy delivered to the zero'th atom. The response to a force distributed in time may be obtained by representing the force as a series of delta-functions of time. The important point however is that the force component on the s'th mode is proportional to $\cos(s\pi/2N)$ and therefore the higher frequency normal modes are not easily excited by a force acting on the end atom of a chain. If the force had been applied to the r'th atom where r is fairly large then the factor $\cos(s\pi/2N)$ would have been replaced by $\cos(r + 1/2) s\pi/N$. This new factor fluctuates rapidly as s is altered so that there would now be no systematic difference between the ease of excitation of low and high frequency modes.

ONE DIMENSIONAL CONTINUUM MODEL

Consider a thin rod of length L, with position along it measured by the coordinate x, $0 \leqslant x \leqslant L$. If $u(x)$ is the longitudinal displacement of the element normally at x then the displacement associated with the s'th normal mode is

$$u_s(x) = A_s \sin \omega_s t \cos \frac{s\pi x}{L} \qquad (A1\text{-}9)$$

and the associated energy is $MA_s^2 \omega_s^2/4 (s \neq 0)$, where M is the total mass of the rod. The corresponding amplitude of motion of the end at $x = 0$, is A_s, so that for a force applied at $x = 0$, the normal mode behaves like an oscillator of mass $M/2$. This result is true of a continuum, but if one attempts to approximate to a lattice by a "Debye" cutoff, i.e. by considering only the first N modes (only unidirectional motion is considered), then an error is made. In particular an impulse I would deliver an energy I^2/M to each mode, or a total of I^2/m to the whole rod, which is twice the correct energy transfer. Perhaps the simplest way to resolve the discrepancy is to consider that when the continuum is to represent a lattice, the force applied to a surface atom must be applied to the continuum not at $x = 0$ but at $x = L/2N$, i.e. one-half of a "lattice spacing" in from the end.
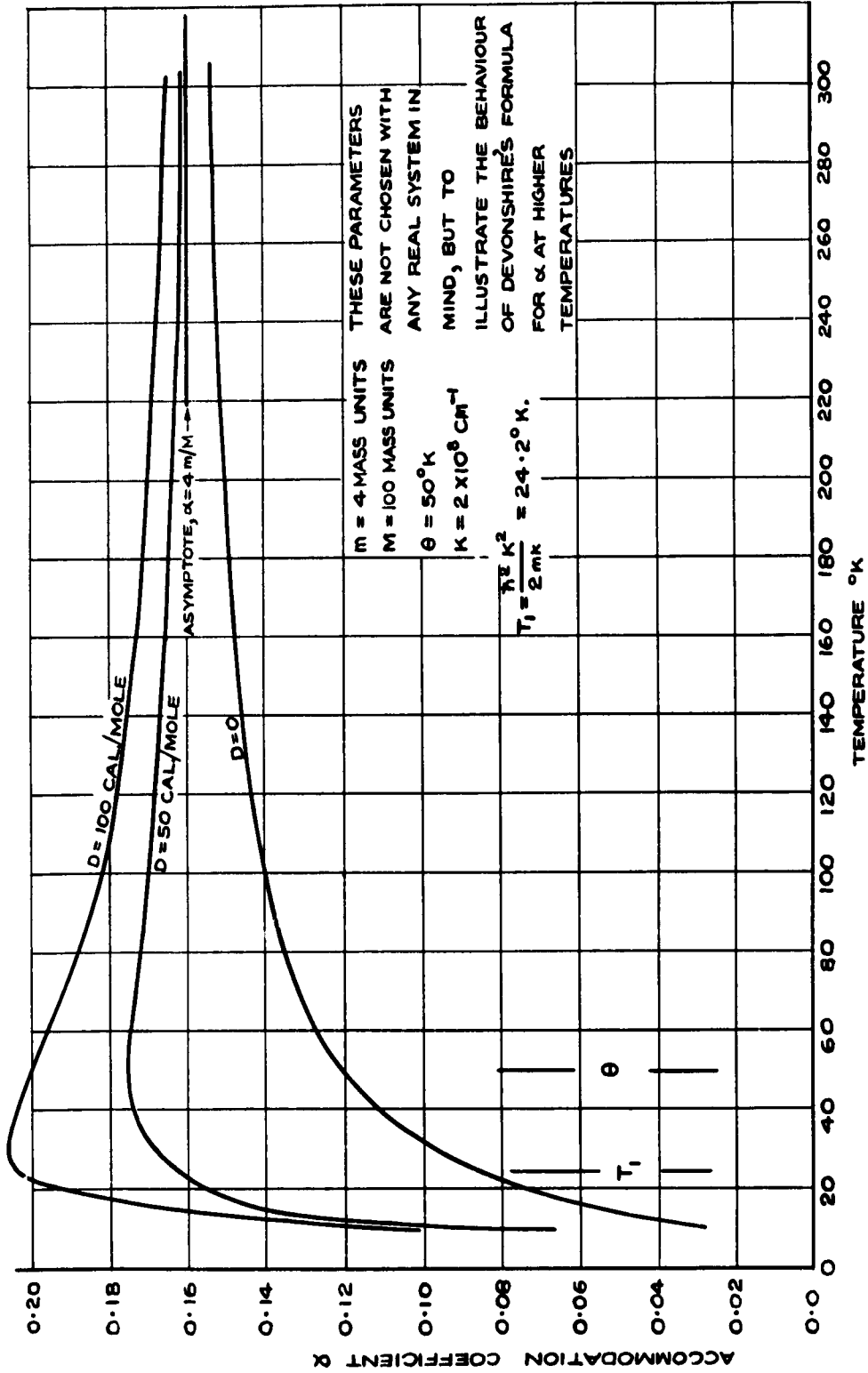
ACCOMMODATION COEFFICIENT α

ASYMPTOTE, $\alpha = 4\,m/M \rightarrow$

D = 100 CAL/MOLE

D = 50 CAL/MOLE

D = 0

m = 4 MASS UNITS   THESE PARAMETERS
M = 100 MASS UNITS   ARE NOT CHOSEN WITH
                       ANY REAL SYSTEM IN
θ = 50° K   MIND, BUT TO
K = 2 × 10⁸ CM⁻¹   ILLUSTRATE THE BEHAVIOUR
                       OF DEVONSHIRE'S FORMULA
$T_1 = \dfrac{\hbar^2 K^2}{2\,mx}$ = 24.2° K.   FOR α AND AT HIGHER
                       TEMPERATURES

θ

T_1

TEMPERATURE °K

FIG.I ACCOMMODATION COEFFICIENTS FROM DEVONSHIRE'S FORMULA,
       SHOWING ASYMPTOTIC BEHAVIOUR.

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